

Accelerated inference with neural networks and agents for Cosmic Microwave Background and Large Scale Structure analyses

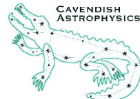
Boris Bolliet

Cavendish Astrophysics and Kavli Institute for Cosmology, Cambridge

Work in collaboration with:

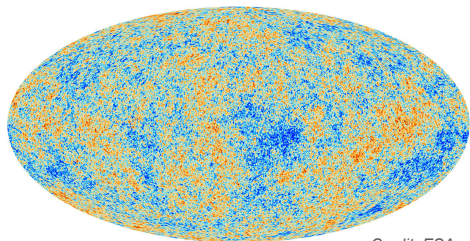
(Neural nets:) Kristen Surrao, Frank Qu, Hidde Jense, Colin Hill, Julien Lesgourgues, Alessio Spurio Mancini, Blake Sherwin

(Agents:) Andrew Laverick, Inigo Zubeldia, Miles Cranmer, Julien Lesgourgues, Antony Lewis, Blake Sherwin



CMB and LSS

Observations



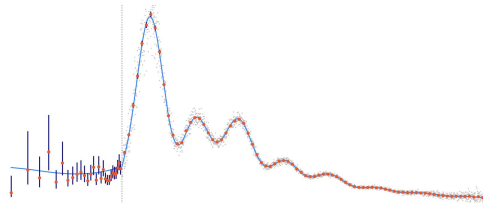
CMB temperature map



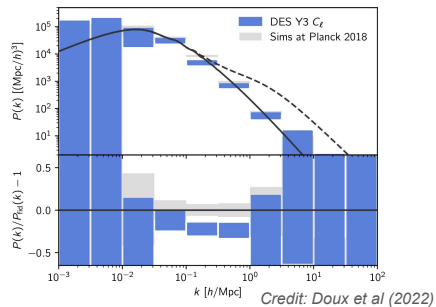
Galaxy surveys

.....

Summary Statistics



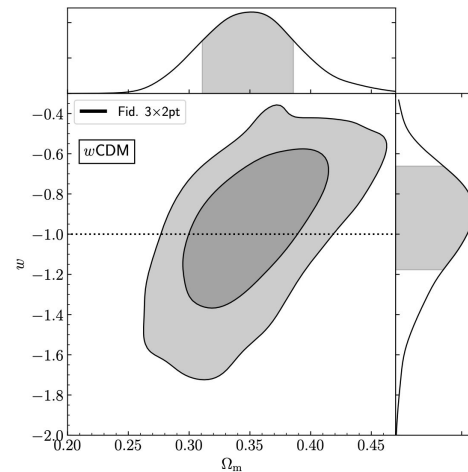
CMB power spectrum



Matter power spectrum

.....

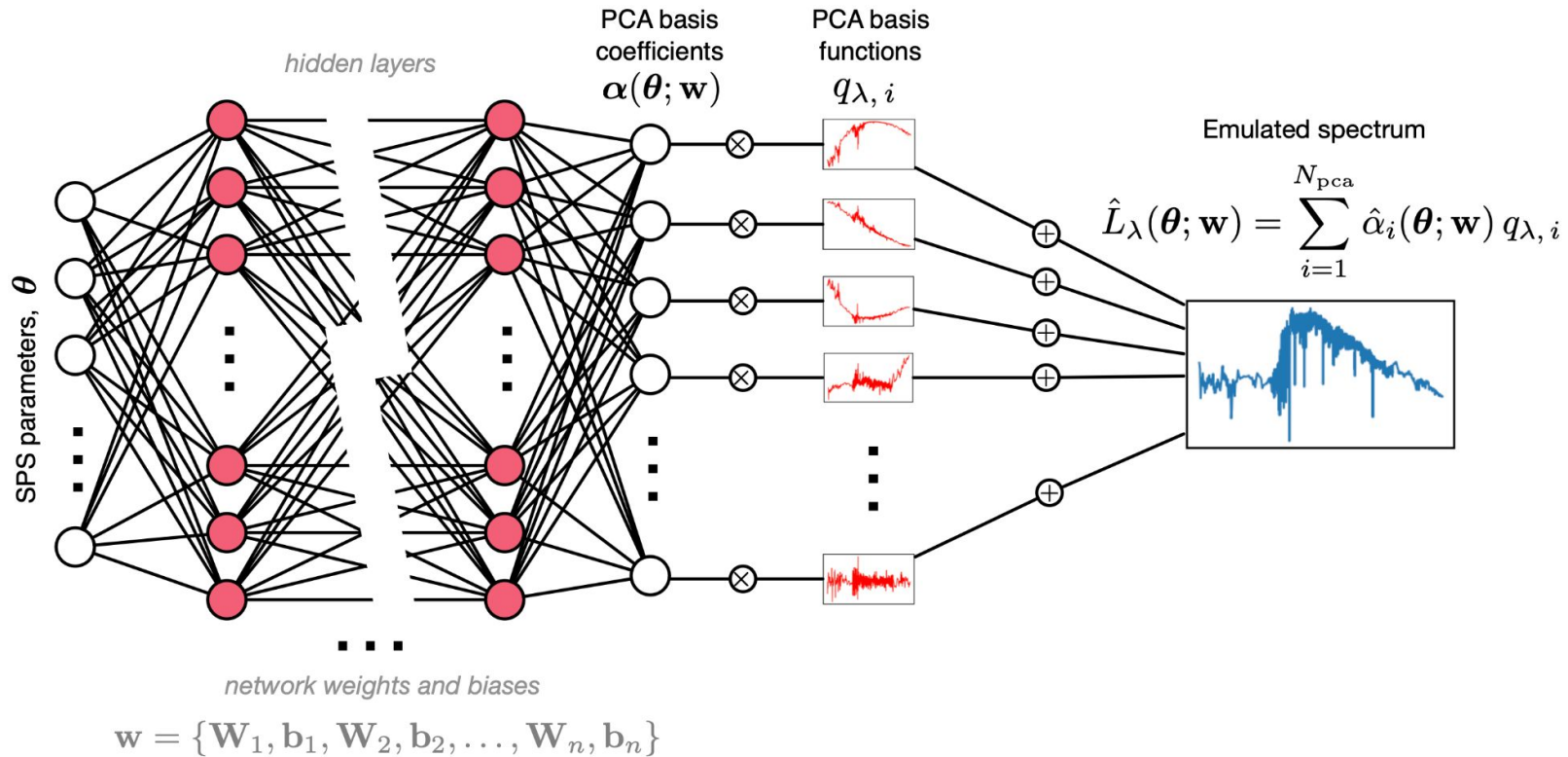
Inference



Parameters
and
Model selection

Neural network emulators

Alsing et al (2020)



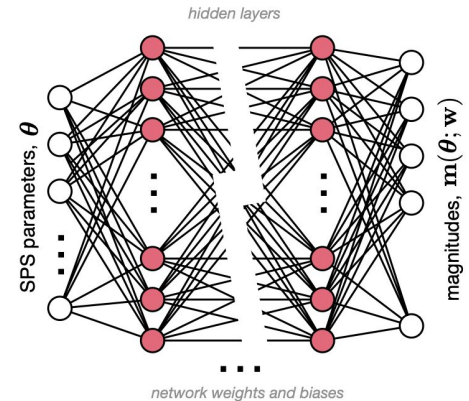
Neural network emulators

Alsing et al (2020), Spurio Mancini et al (2020)

- Fully connected neural net with $n=4$ hidden layers
- 512 neurons per layer
- Activation function

$$f(\mathbf{x}) = \left(\gamma + \left(1 + e^{-\beta \odot \mathbf{x}} \right)^{-1} \odot (1 - \gamma) \right) \odot \mathbf{x}$$

- Adam optimizer
- L2 loss



$$\mathbf{w} = \{\mathbf{W}_1, \mathbf{b}_1, \mathbf{W}_2, \mathbf{b}_2, \dots, \mathbf{W}_n, \mathbf{b}_n\}$$

$$\begin{aligned} \hat{\mathbf{m}}(\theta; \mathbf{w}) &= a_n(\mathbf{W}_n \mathbf{y}_{n-1} + \mathbf{b}_n), \\ \mathbf{y}_{n-1} &= a_{n-1}(\mathbf{W}_{n-1} \mathbf{y}_{n-2} + \mathbf{b}_{n-1}) \\ &\vdots \\ \mathbf{y}_1 &= a_1(\mathbf{W}_1 \theta + \mathbf{b}_1), \end{aligned}$$

Training/testing set generation (i.e., simulations)

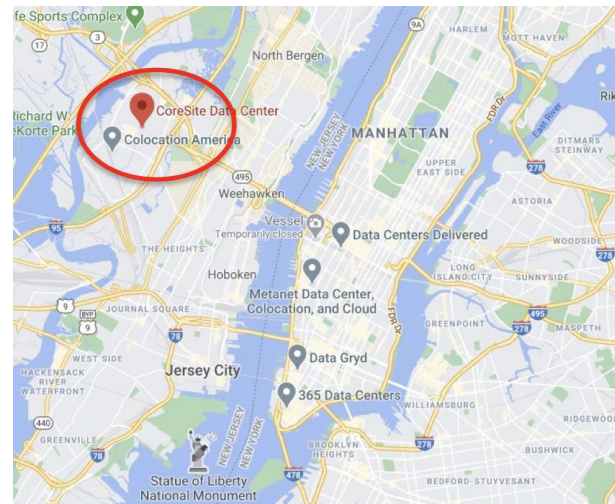
- On AMD Rome nodes
- Maximally/optimally distributed and parallelized

An N=500 job array

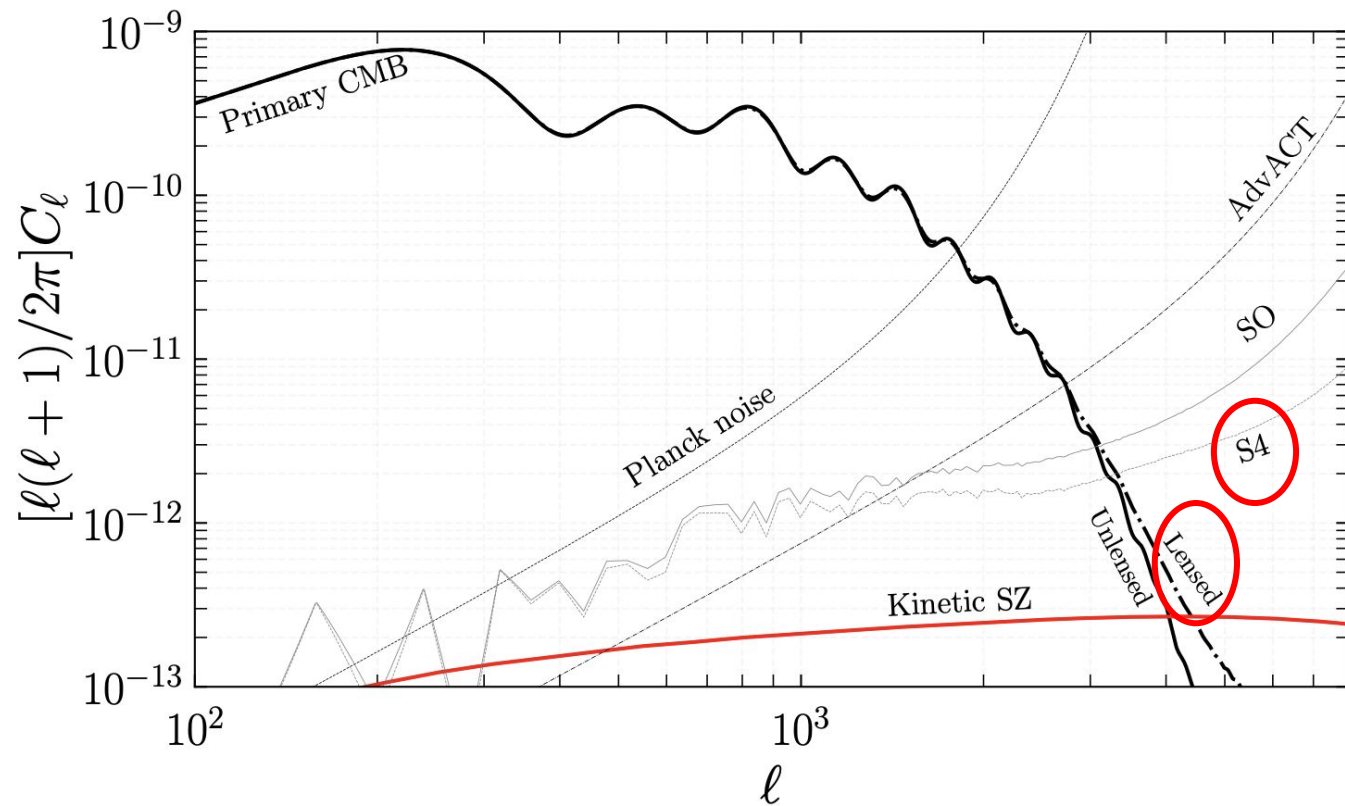
Each job: 1k simulations

Each simulations: 128 cores

- Run time ~ 1 week
- Output: 500k realizations of each observable/spectra
- All project so far: 1.5TB of training data



CMB/LSS in stage 4 era



High accuracy and precision

- Aim for **Stage IV** cosmological surveys

$$\ell = 10\,000$$

•

$$k = 50 h/\text{Mpc}$$

$$z = 20$$

- State-of-the-art **baryonic**, **recombination** and **BBN** physics

 [HMcode](#) Public

Augmented halo model for accurate non-linear matter power spectrum calculations

Mead et al (2020)

 [HYREC-2](#) Public

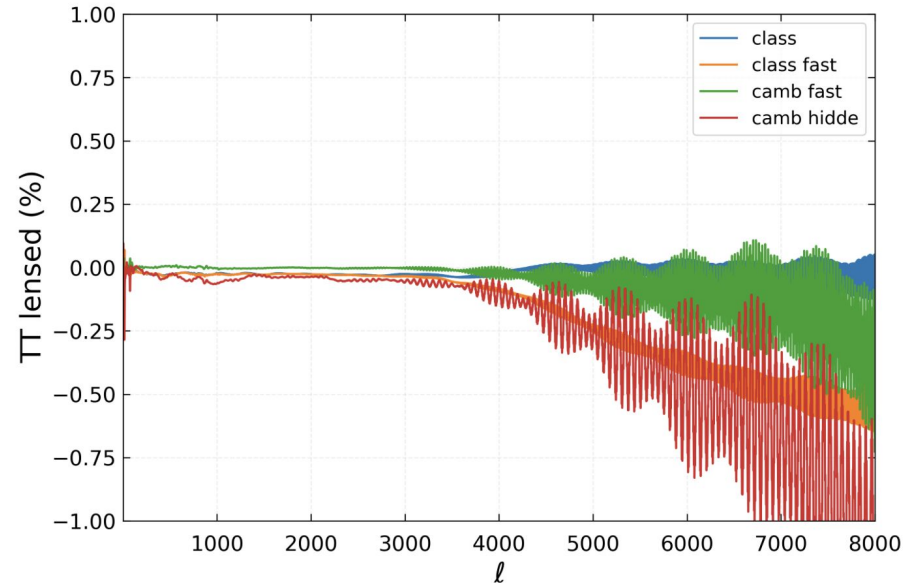
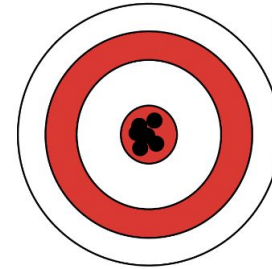
A code for cosmological recombination history (arXiv:2007.14114)

Lee & Ali-Haïmoud (2020)

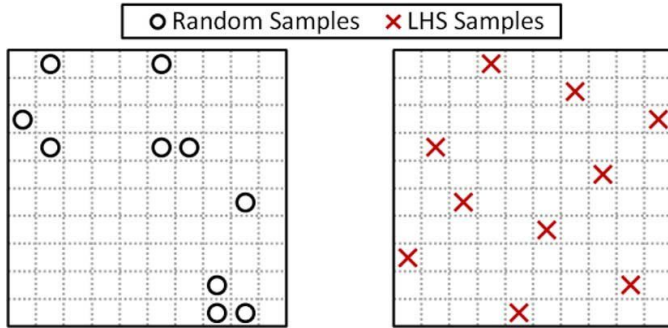
PRIMAT

PRImordial MATter

Pitrou et al (2019)



Latin Hypercube of parameters



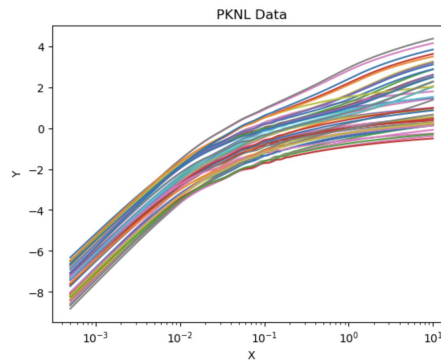
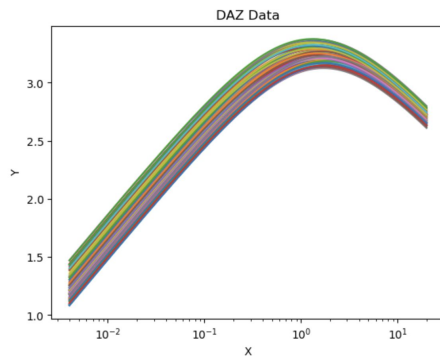
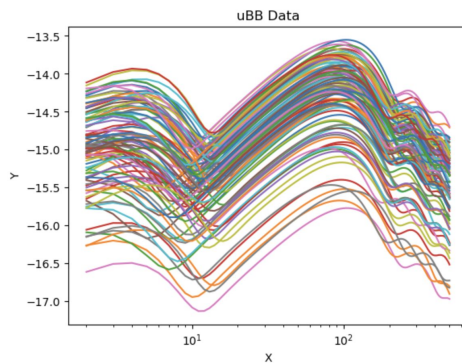
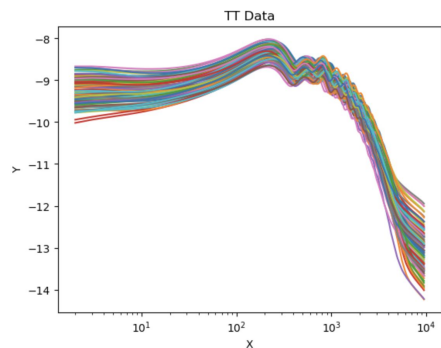
- N=12 dimension
- Priors wide enough for all commonly used datasets

	fEDE	log10z_c	thetai_scf	ln10 ^{10} A_s	n_s	H0	omega_b	omega_cdm	r	m_ncdm	N_ur	tau_reio
count	101.000000	101.000000	101.000000	101.000000	101.000000	101.000000	101.000000	101.000000	101.000000	101.000000	101.000000	101.000000
mean	0.278861	3.595969	1.527791	2.967161	0.997687	71.556618	0.022533	0.133713	0.147924	0.144726	0.428654	0.074669
std	0.138575	0.361907	0.870957	0.293460	0.122244	16.471014	0.001716	0.033989	0.091031	0.090054	1.264378	0.026748
min	0.011895	3.009630	0.105130	2.500174	0.804327	40.199589	0.019422	0.080967	0.002438	0.000773	-1.990748	0.020113
25%	0.164462	3.296597	0.790361	2.737349	0.888013	59.010735	0.021174	0.107319	0.066991	0.076257	-0.611414	0.053747
50%	0.279028	3.603682	1.514083	2.956763	0.988622	72.493774	0.022748	0.129041	0.160872	0.132455	0.428871	0.076161
75%	0.390485	3.922711	2.199476	3.187469	1.113980	85.024414	0.024234	0.163343	0.222737	0.214756	1.480172	0.096894
max	0.499414	4.268420	3.094030	3.484036	1.192105	98.807076	0.025310	0.198256	0.294089	0.320833	2.499874	0.119843

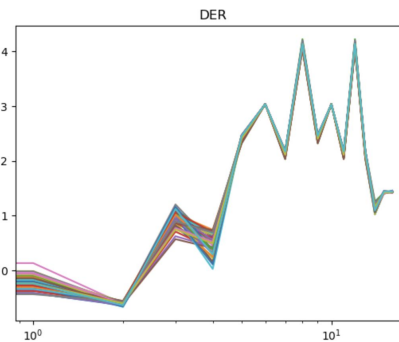
EDE

LCDM

Training/testing sets



- Curse of dimensionality: np.interp need $\sim 10^d$ samples, memory and computing time impossible
- Neural nets nail it



Training of neural net

- On NVIDIA H100 GPUs at Flatiron Institute
- GPU job array (each job train for 1 observable)

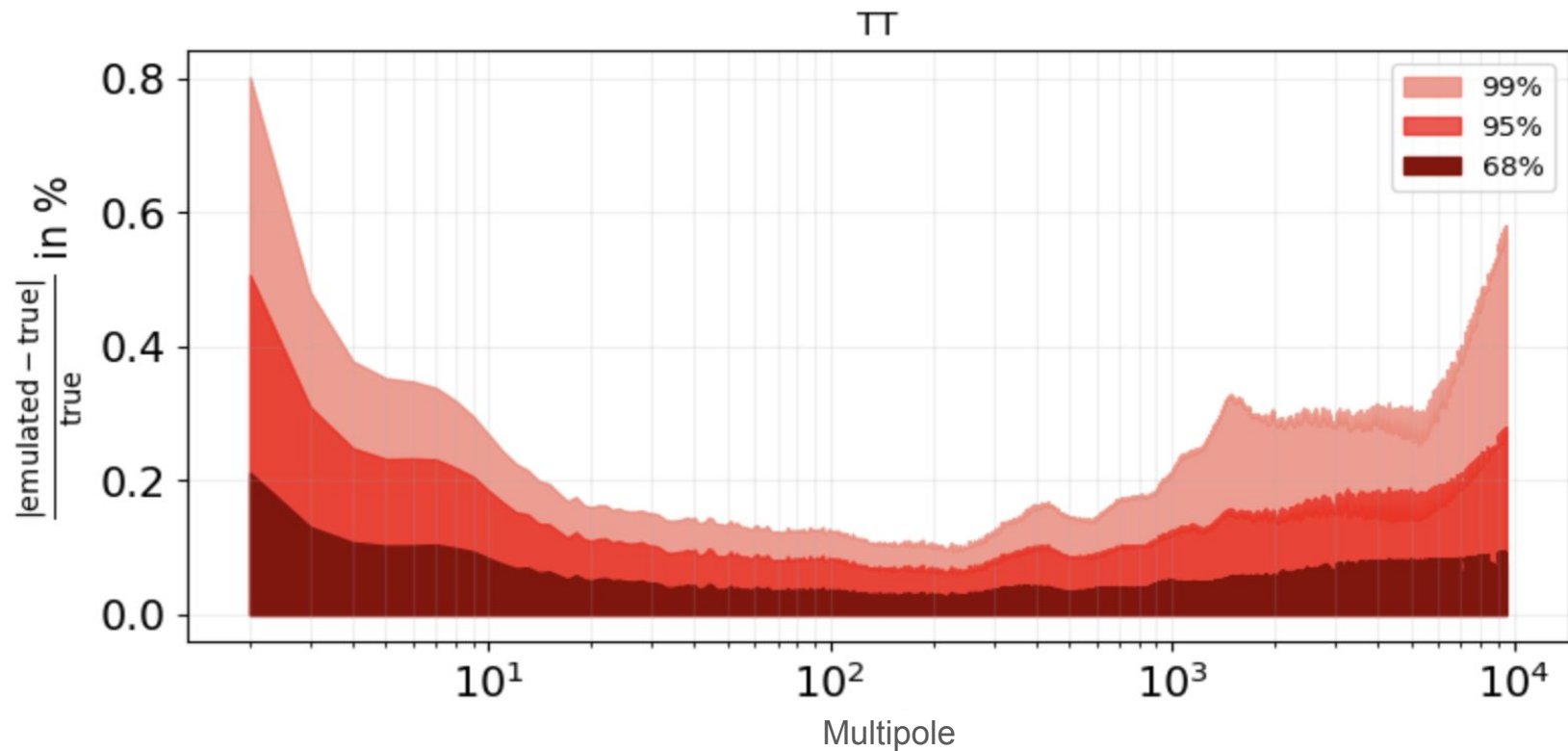
```
l_func_obstypes = ['TT', 'TE', 'EE', 'BB', 'uTT', 'uTE', 'uEE', 'uBB', 'PP']
k_func_obstypes = ['PKL', 'PKLCB', 'PKNL', 'PKNLCB']
z_func_obstypes = ['S8Z', 'HZ', 'DAZ']
```

- Cosmopower training strategy

```
cp_nn.train(training_parameters=training_parameters,
            training_features=training_features,
            filename_saved_model=hmdir+'%s'%VAR,
            validation_split=0.1,
            learning_rates=[1e-2, 1e-3, 1e-4, 1e-5, 1e-6],
            batch_sizes=[1024, 1024, 1024, 1024, 1024],
            gradient_accumulation_steps = [1, 1, 1, 1, 1],
            # early stopping set up
            patience values = [100,100,100,100,100],
            max_epochs = [1000,1000,1000,1000,1000])
```

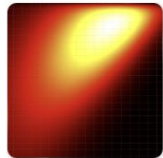


Diagnostic

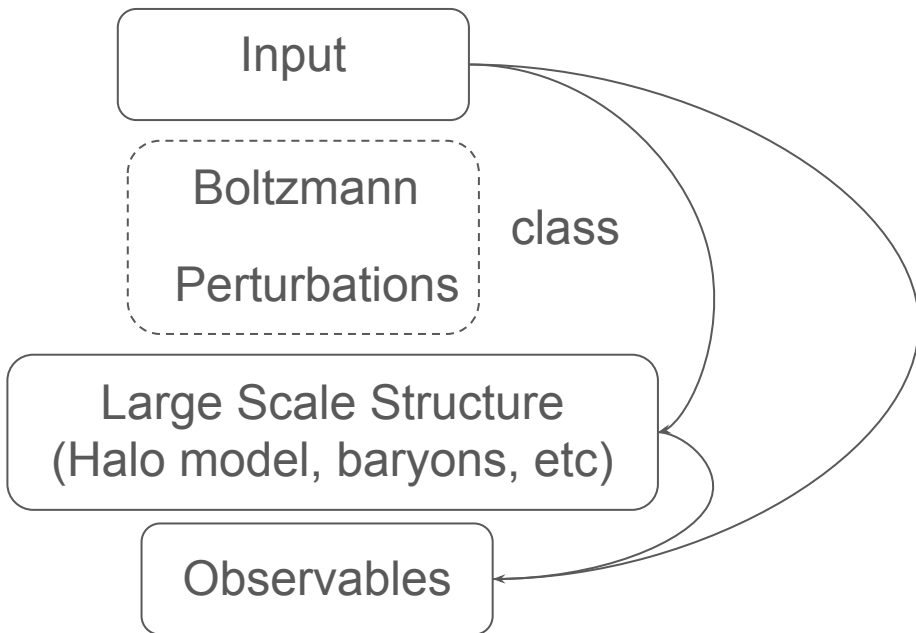


- Is this the best architecture?
- Data challenge, stay tuned!

Packaging @ <https://github.com/CLASS-SZ>

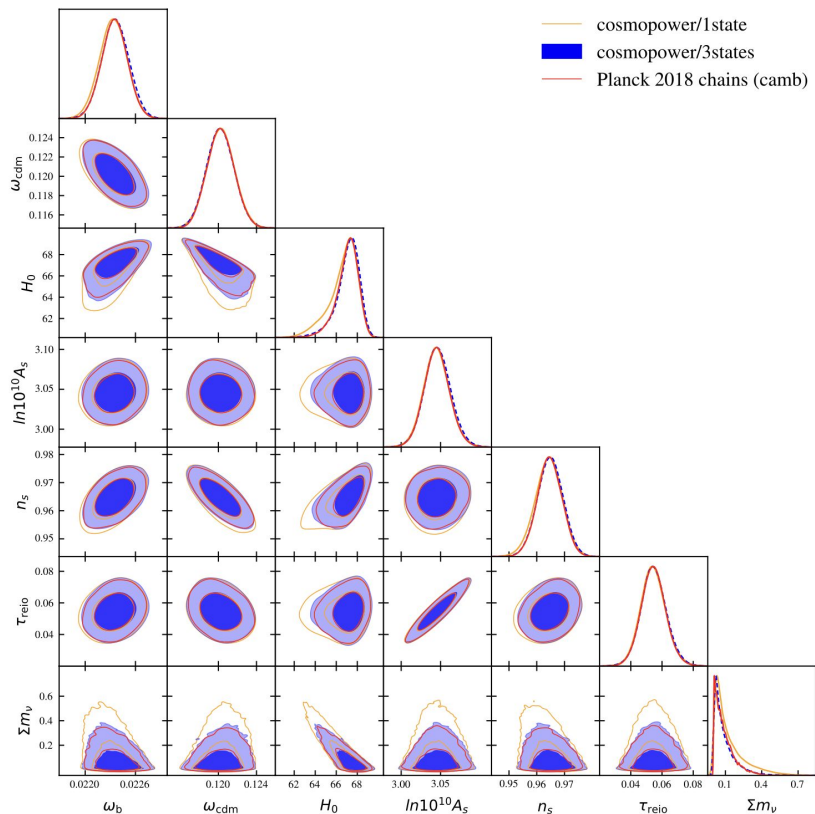


Machine Learning accelerated CMB & LSS calculations



- Bypass slow parts of Boltzmann solver
- Substitute emulated quantities
- Compute LSS observables
- Readily compatible with MCMC codes like `cobaya`

Performance



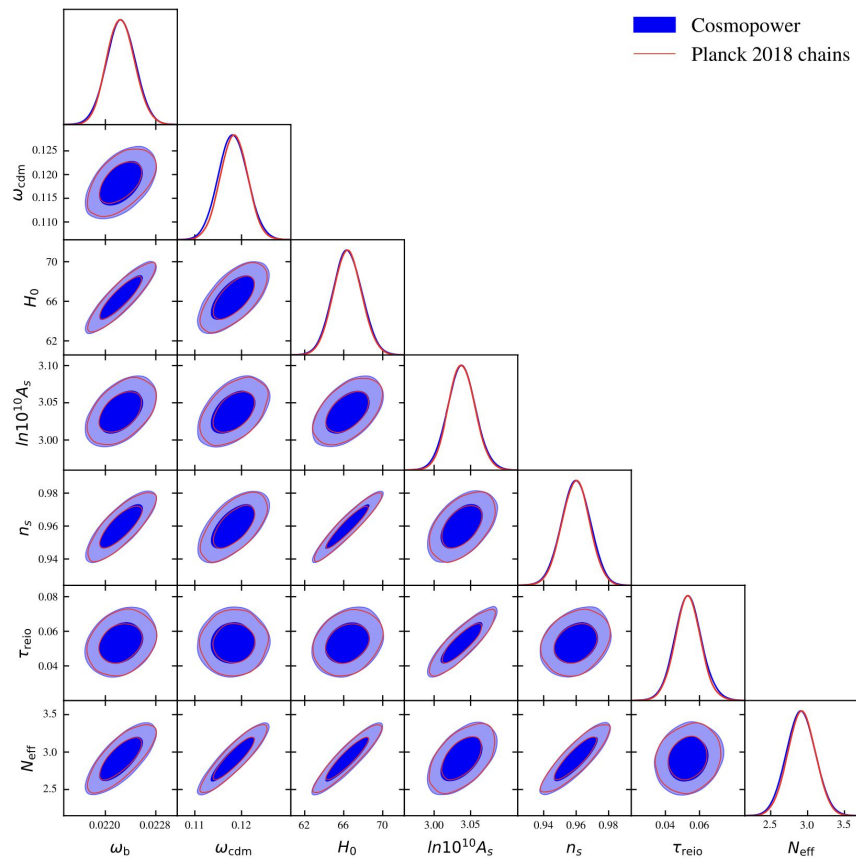
Massive neutrinos

$$M_\nu$$

<https://github.com/cosmopower-organization/mnu-3states>

MCMC analysis in minutes on a laptop

Performance



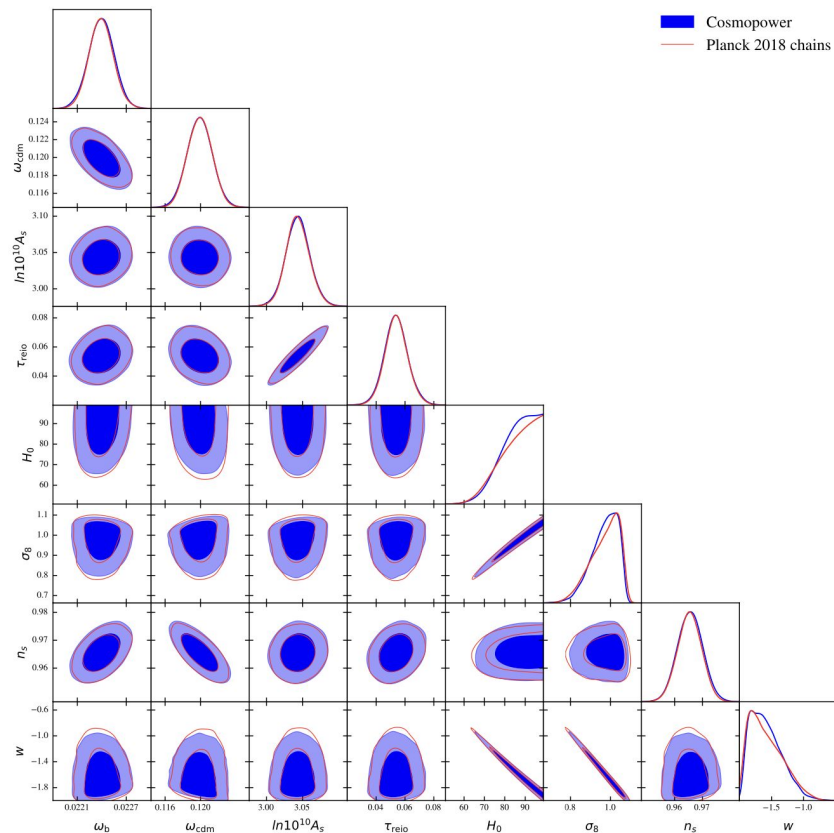
Effective number of relativistic species

$$N_{\text{eff}}$$

<https://github.com/cosmopower-organization/neff>

MCMC analysis in minutes on a laptop

Performance



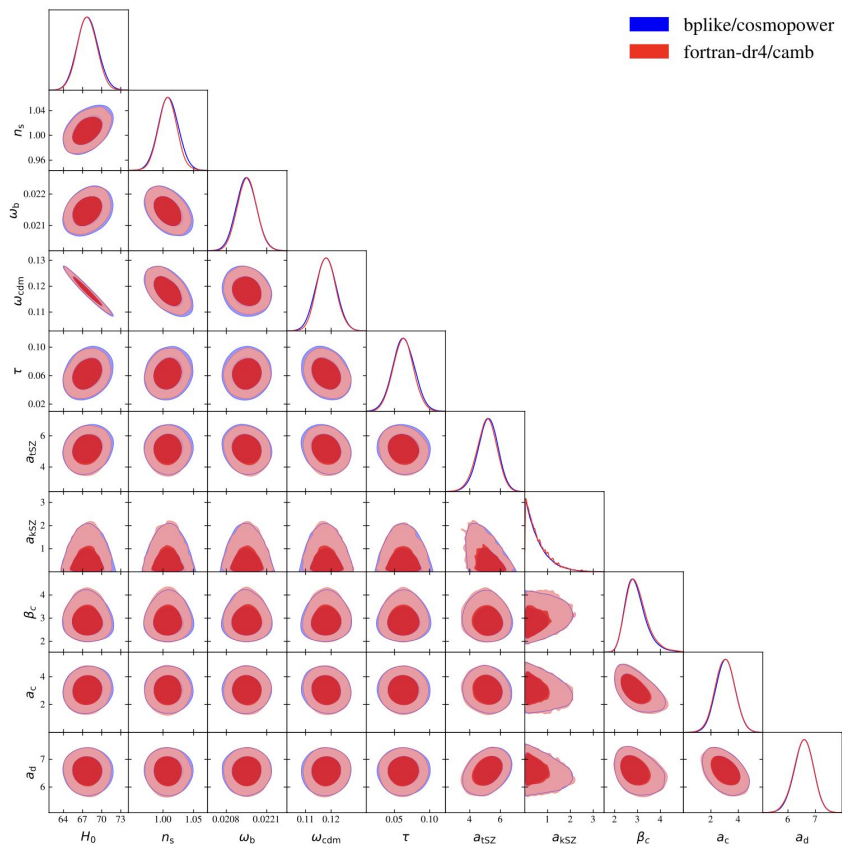
Dark energy

w

<https://github.com/cosmopower-organization/wcdm>

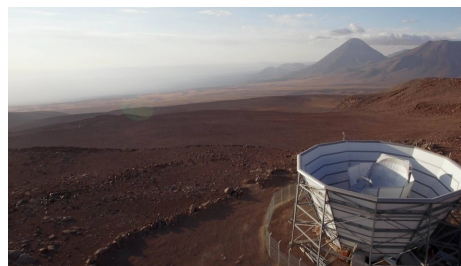
MCMC analysis in minutes on a laptop

Performance



ACT DR4

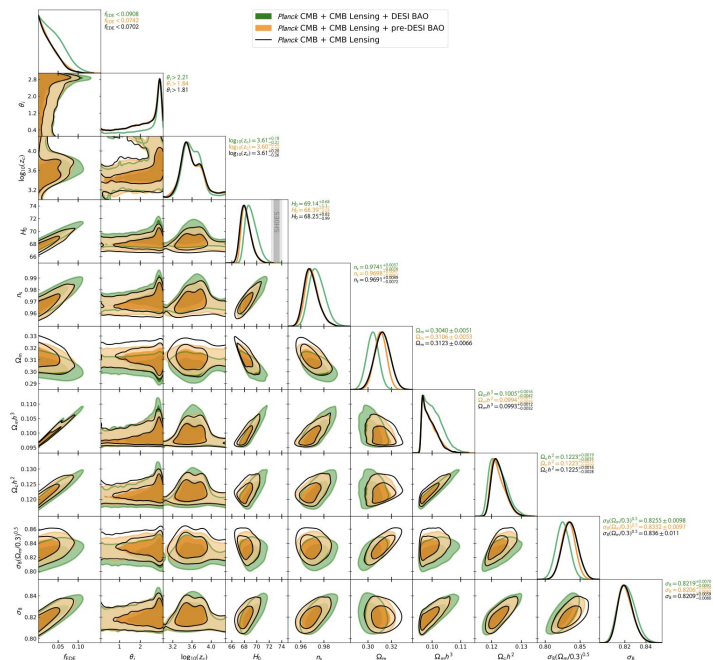
Choi et al (2020)



MCMC analysis in minutes on a laptop

Application to EDE constraints

- DESI DR1: April 3rd 2024
- (Qu, Surrao, Bolliet et al 2024:) April 25th 2024, more than 20 MCMCs, impossible without emulators (or take ~ 6 months to 1 year)



Kristen Surrao
Columbia

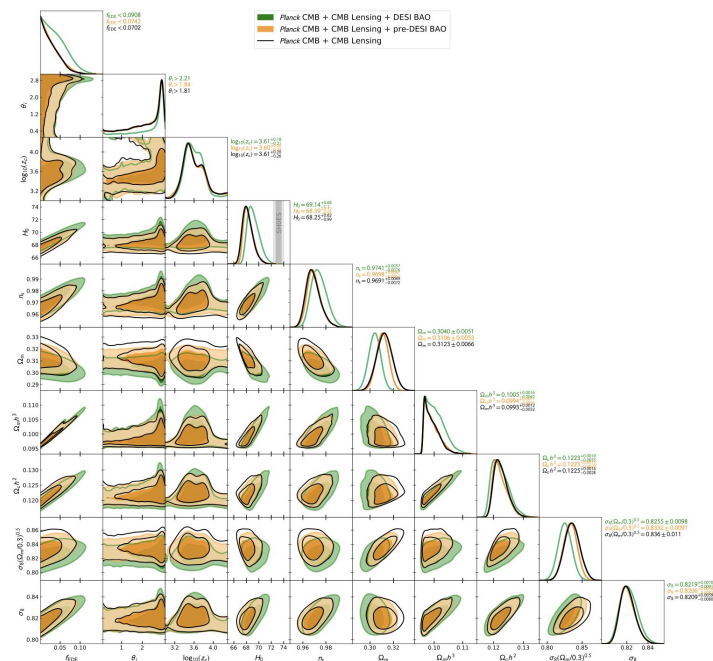


Frank Qu
Cambridge

<https://github.com/cosmopower-organization/ede>

Application to EDE constraints

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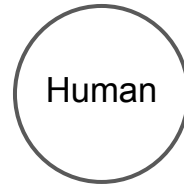
Kristen Surrao
Columbia



Frank Qu
Cambridge

Time is precious.... Do we really need to spend so much of it setting-up and running mcmc's?

Inference with agents

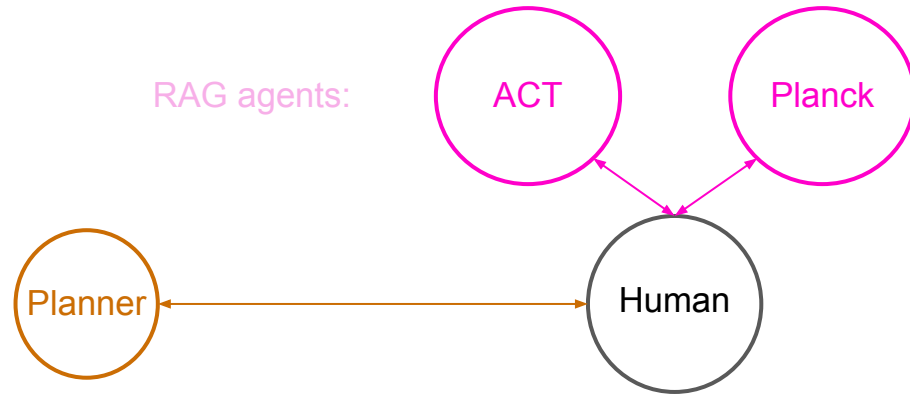


Inference with agents



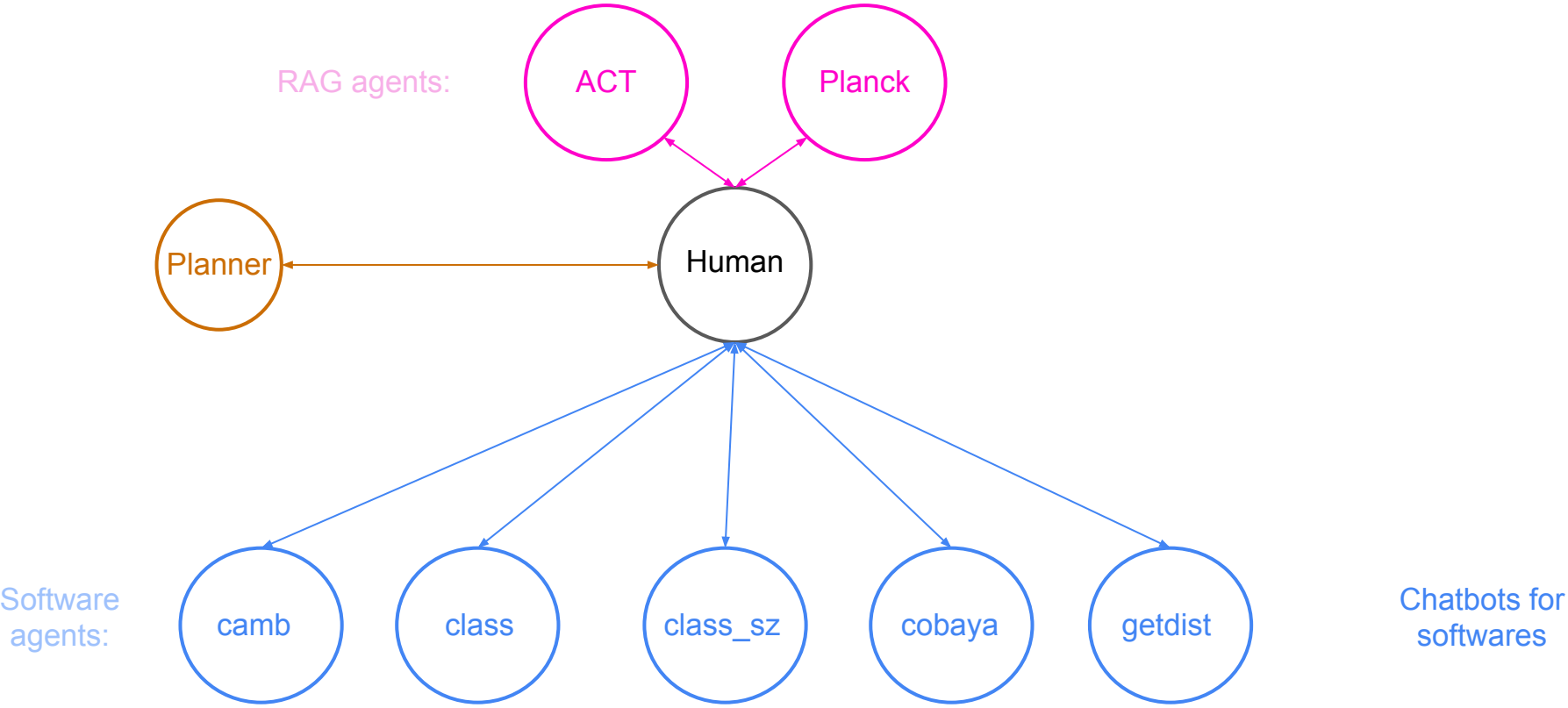
Make a plan

Inference with agents

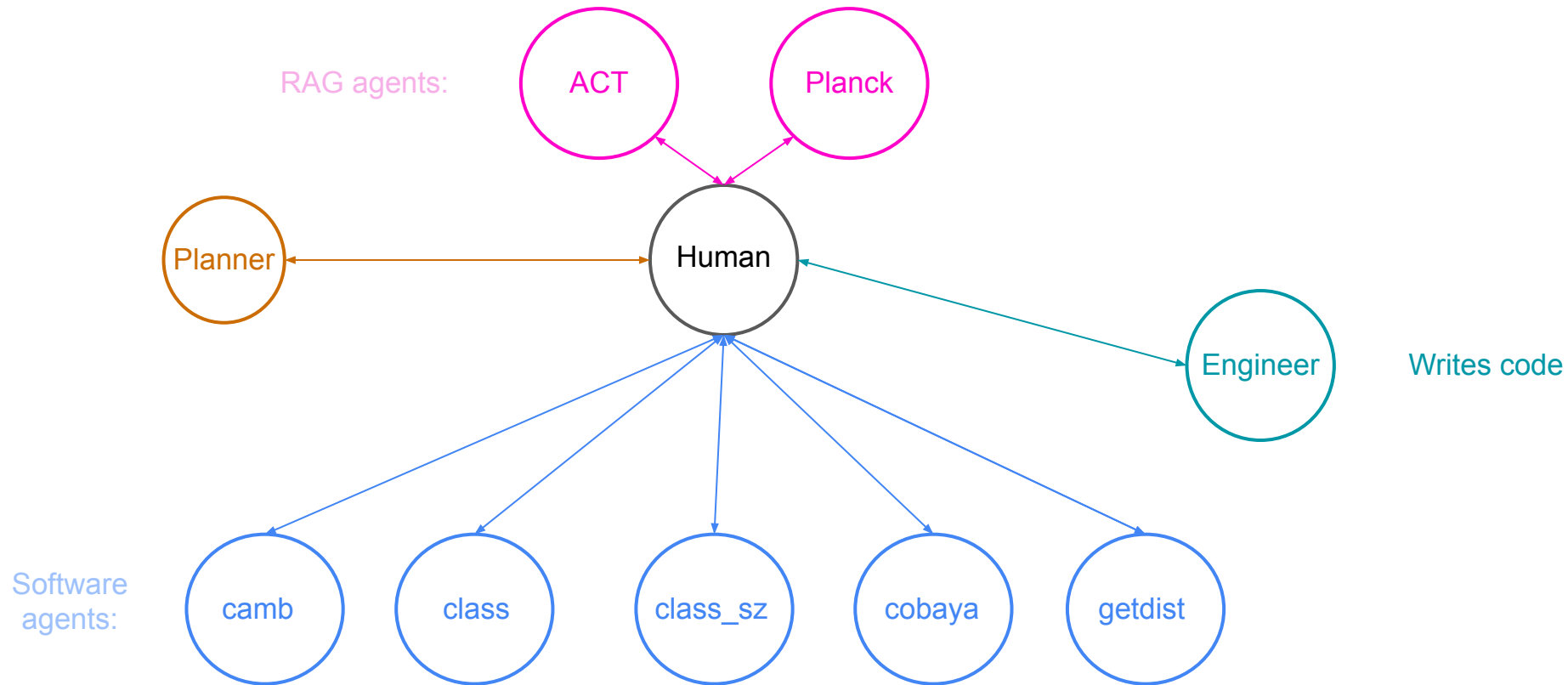


Retrieve info from
collaboration papers and
codes

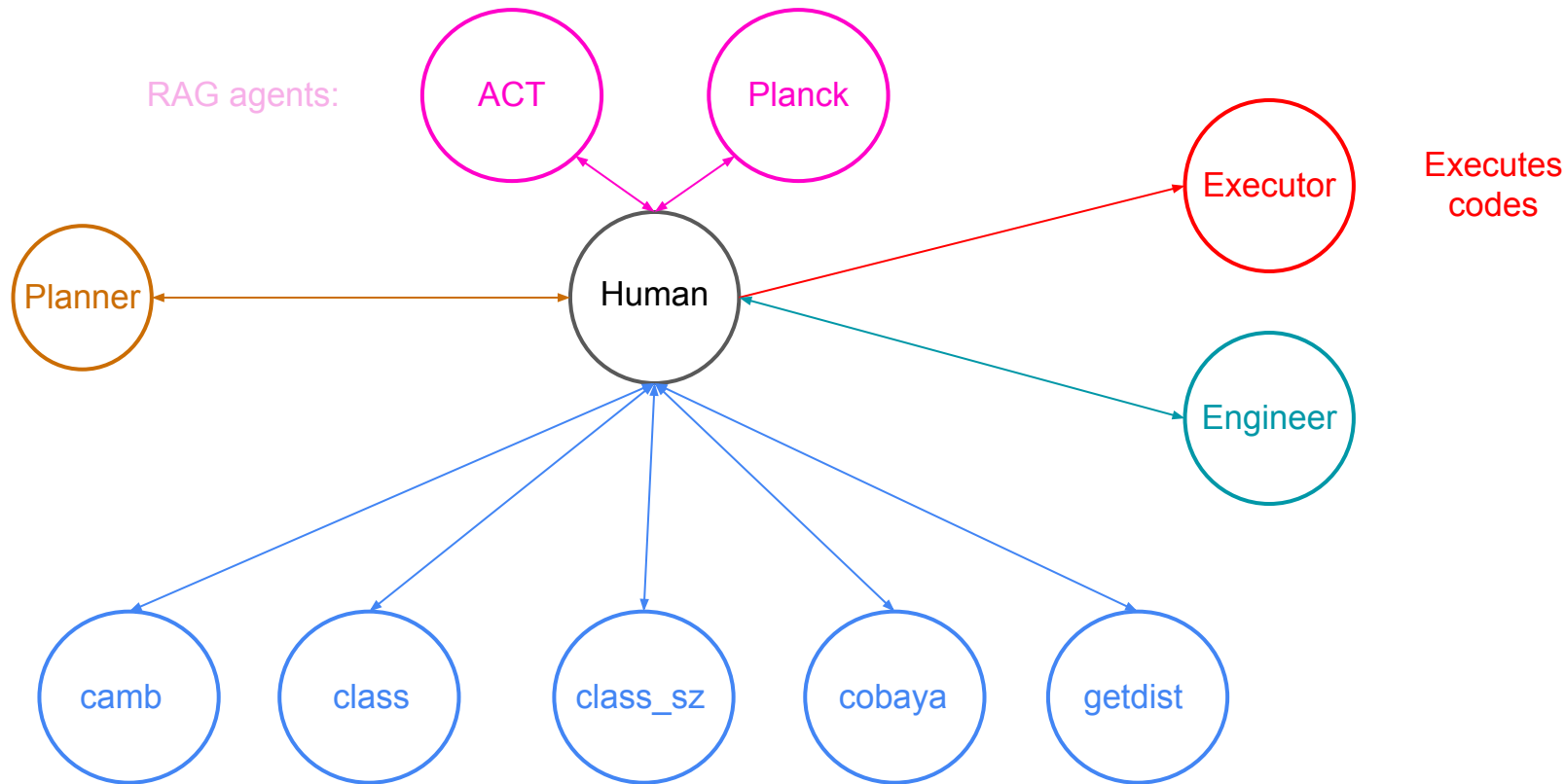
Inference with agents



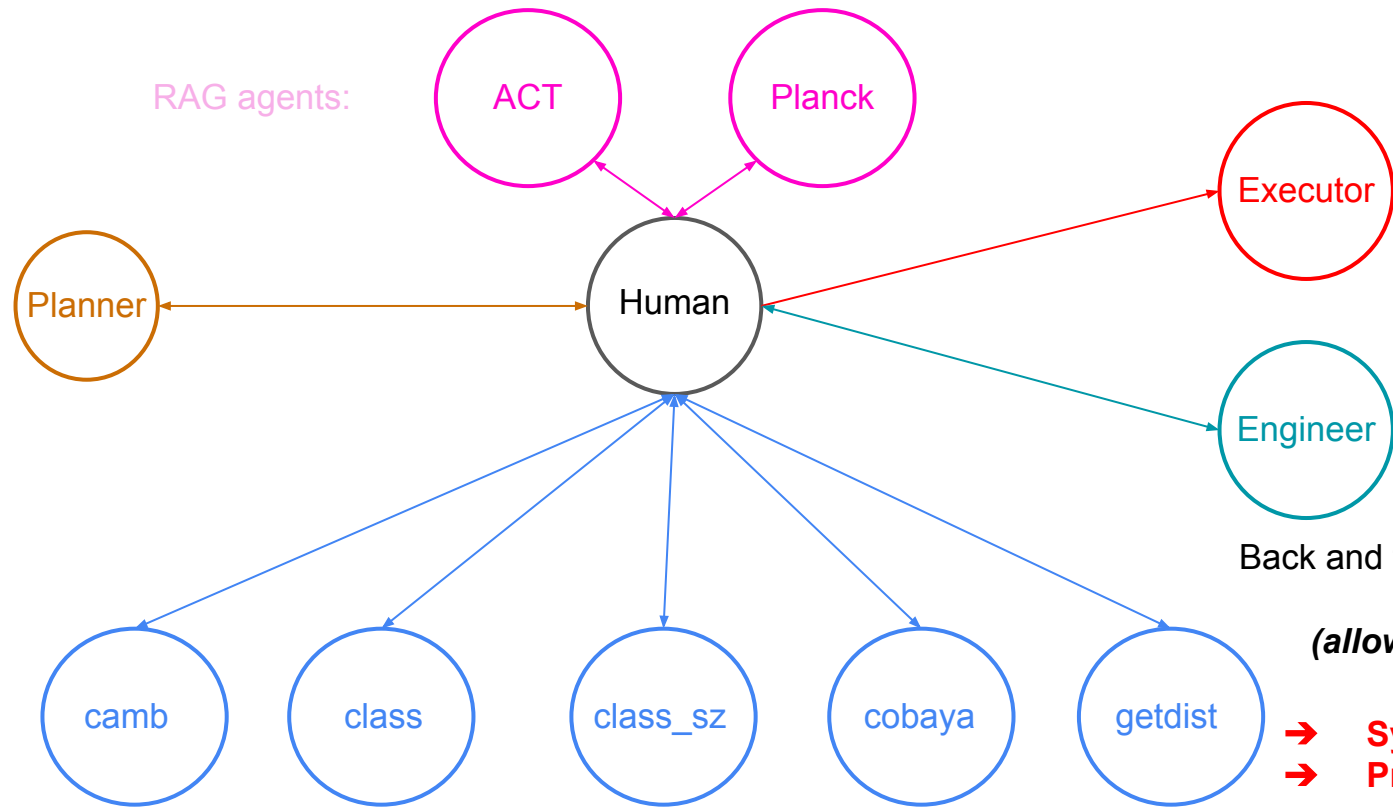
Inference with agents



Inference with agents



Inference with agents



RAG agents:

ACT

Planck

Planner

Human

Executor

Engineer

camb

class

class_sz

cobaya

getdist

Back and forth between human and agents
(allowed transitions)

Software agents:

→ **System engineering**
→ **Prompt engineering**

Inference with agents

Task 1: Evaluate act_dr6_lenslike likelihood at given σ_8 and Ω_m values

```
message="""  
  Get cosmological paramater values from Planck 2018 analysis of TT,TE,EE+lowE+lensing with the Plik likelihood in LCDM.  
  Use cobaya with classy_sz to evaluate the ACT DR6 lensing likelihood for sigma8=0.8 and Omega_m=0.31. Other parameters set to Planck 2018.  
  To set Omega_m, adjust the value of omch2.  
  Give me the value of log-likelihood.  
  Instructions: First make a plan. Then follow the plan once admin gives green-light. The plan may be modified in the process. In case of modification, always print the full updated plan.  
"""
```

Inference with agents

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Make plan

Inference with agents

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"""
```

Next speaker: planner

planner (to chat_manager):

Plan to Get Cosmological Parameter Values and Evaluate ACT DR6 Lensing Likelihood

Step 1: Retrieve Cosmological Parameter Values from Planck 2018 Analysis

- 1.1 **Retrieve Planck 2018 Cosmological Parameters:**
 - **Responsible Agent:** planck_agent
 - **Details:** Retrieve the cosmological parameter values from the Planck 2018 analysis of TT,TE,EE+lowE+lensing with the Plik likelihood in LCDM.
- 1.2 **Review Retrieved Parameters:**
 - **Responsible Agent:** admin
 - **Details:** Admin reviews the retrieved parameters to ensure they are correct.

Step 2: Set Up Cobaya with Classy_sz to Evaluate ACT DR6 Lensing Likelihood

- 2.1 **Set Up YAML File for Cobaya:**
 - **Responsible Agent:** cobaya_agent
 - **Details:** Suggest how to set up the YAML file for Cobaya to use the Planck 2018 parameters and adjust omch2 to achieve $\Omega_m=0.31$ and $\sigma_8=0.8$.
- 2.2 **Write Code to Run Cobaya with Classy_sz:**
 - **Responsible Agent:** engineer
 - **Details:** Write the code to run Cobaya with Classy_sz using the YAML file.
- 2.3 **Run Cobaya with Classy_sz:**
 - **Responsible Agent:** executor
 - **Details:** Execute the code to run Cobaya with Classy_sz.
- 2.4 **Review Cobaya Run Results:**
 - **Responsible Agent:** admin
 - **Details:** Admin reviews the results of the Cobaya run to ensure they are correct.

Step 3: Evaluate ACT DR6 Lensing Likelihood

- 3.1 **Evaluate ACT DR6 Lensing Likelihood:**
 - **Responsible Agent:** classy_sz_agent
 - **Details:** Suggest how to evaluate the ACT DR6 lensing likelihood for the given parameters.
- 3.2 **Write Code to Evaluate ACT DR6 Lensing Likelihood:**
 - **Responsible Agent:** engineer
 - **Details:** Write the code to evaluate the ACT DR6 lensing likelihood.



Make plan

Inference with agents

Task 1: Evaluate act_dr6_lenslike likelihood at given σ_8 and Ω_m values

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Give me the value of log-likelihood.  
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"""
```

Execute

Inference with agents

Task 1: Evaluate act_dr6_lenslike likelihood at given σ_8 and Ω_m values

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Give me the value of log-likelihood.
Instructions: First make a plan. Then follow the plan once admin gives green-light. The plan may be modified in the process. In case of modification, always print the full updated plan.
"""
```

Next speaker: executor

```
>>>>>> EXECUTING CODE BLOCK (inferred language is python)...
executor (to chat_manager):
```

```
exitcode: 0 (execution succeeded)
Code output: [output] Output to be read-from/written-into folder '.', with prefix 'cobaya_config'
[output] Found existing info files with the requested output prefix: 'cobaya_config'
[output] Will delete previous products ('force' was requested).
[classy_szfast.classy_sz.classy_sz] Initialized!
[evaluate] *WARNING* No sampled parameters requested! This will fail for non-mock samplers.
[evaluate] Initialized!
[evaluate] Looking for a reference point with non-zero prior.
[evaluate] Reference point:

[evaluate] Evaluating prior and likelihoods...
[evaluate] log-posterior = -8.74847
[evaluate] log-prior      = 0
[evaluate]   logprior_0 = 0
[evaluate] log-likelihood = -8.74847
[evaluate]   chi2_act_dr6_lenslike.ACTDR6LensLike = 17.4969
[evaluate] Derived params:
[act_dr6_lenslike.actdr6lenslike] Average evaluation time for act_dr6_lenslike.ACTDR6LensLike: 0.0832734 s (1 evaluations)
[classy_szfast.classy_sz.classy_sz] Average evaluation time for classy_szfast.classy_sz.classy_sz: 0.0287849 s (1 evaluations)
```



Execute

Inference with agents

Task 1: Evaluate act_dr6_lenslike likelihood at given σ_8 and Ω_m values

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```

Report

Inference with agents

Task 1: Evaluate act_dr6_lenslike likelihood at given σ_8 and Ω_m values

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Use cobaya with classy_sz to evaluate the ACT DR6 lensing likelihood for sigma8=0.8 and Omega_m=0.31. Other parameters set to Planck 2018.
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Give me the value of log-likelihood.
Instructions: First make a plan. Then follow the plan once admin gives green-light. The plan may be modified in the process. In case of modification, always print the full updated plan.
""
```

```
Next speaker: planner
planner (to chat_manager):

### Initial Goal

The initial goal was to:
1. **Retrieve Cosmological Parameter Values from Planck 2018 Analysis:**
  - Get cosmological parameter values from Planck 2018 analysis of TT,TE,EE+lowE+lensing with the Plik likelihood in LCDM.
2. **Use Cobaya with Classy_sz to Evaluate the ACT DR6 Lensing Likelihood:**
  - Evaluate the ACT DR6 lensing likelihood for  $(\sigma_8 = 0.8)$  and  $(\Omega_m = 0.31)$  using Cobaya with Classy_sz.
  - Adjust the value of  $(\Omega_{\text{m}}^{\text{ch2}})$  to set  $(\Omega_m)$ .
  - Retrieve the value of the log-likelihood.

### Current Status
- **Step 1:** Retrieve Cosmological Parameter Values from Planck 2018 Analysis (Completed)
- **Step 2:** Set Up Cobaya with Classy_sz to Evaluate ACT DR6 Lensing Likelihood (Completed)
  - **2.1:** Set Up YAML File for Cobaya (Completed)
  - **2.2:** Write Code to Run Cobaya with Classy_sz (Completed)
  - **2.3:** Run Cobaya with Classy_sz (Completed)
  - **2.4:** Review Cobaya Run Results (Completed)

### Results
- **log-likelihood:** -8.74847

### Next Steps
Since the initial goal was to retrieve the log-likelihood value, and we have successfully obtained it, the next steps would be:
1. **Review the Log-likelihood Value:**
  - Ensure the log-likelihood value meets the requirements.
2. **Document and Report:**
  - Document the process and results.
  - Report the findings.

### Summary of Agent Responsibilities:
- **planck_agent:** Retrieve Planck 2018 cosmological parameters. (Completed)
- **cobaya_agent:** Suggest YAML setup for Cobaya. (Completed)
- **classy_sz_agent:** Suggest evaluation method for ACT DR6 lensing likelihood. (Completed)
- **getdist_agent:** Suggest method to retrieve log-likelihood value. (Completed)
- **engineer:** Write code for Cobaya setup, ACT DR6 lensing likelihood evaluation, and log-likelihood retrieval. (Completed)
- **executor:** Run the code for Cobaya setup, ACT DR6 lensing likelihood evaluation, and log-likelihood retrieval. (Completed)
- **admin:** Review all retrieved parameters, results, and values at each step. (Completed)

Please confirm if the log-likelihood value meets the requirements and if we can proceed to document and report the findings.
```



Report

Inference with agents

Task 6: Reproduce the analysis, with BAOs this time - setup yaml file

```
message=""" Set-up a yaml file for cobaya so that we can reproduce the act_dr6_lenslike baseline MCMC analysis with BAOs.
Our theory code is classy_sz.
Follow this plan:
  1. Ask cobaya_agent for input on how to set-up a yaml file that will work with classy_sz as theory code
  2. Ask act_dr6_agent about the BAO likelihoods in example yaml file.
    Adopt the same settings as the example for the act_dr6_lenslike likelihood block.
    Adopt same parameters and priors as in the example yaml file
  3. Ask engineer to make the yaml file
  4. Save the yaml file as /Users/boris/CMBAgents/DataAgent/Coding/chains/dr6_lensing/dr6_lensing_rep.yaml
  5. Show the content of the yaml and ask admin if you can conclude.
"""
```

Write yaml

Inference with agents

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5. Show the content of the yaml and ask admin if you can conclude.
"""
```



```
-----
Next speaker: engineer
engineer (to chat_manager):
## Step 3: Creating the YAML File
Based on the information provided by the 'cobaya_agent' and 'act_dr6_agent', I will create the YAML file for the Cobaya MCMC analysis with 'classy_sz' as the theory code and the specified BAO likelihoods.
Here is the complete Python code to generate the YAML file:
```python
import yaml

data = {
 'theory': {
 'classy_szfast.classy_sz.classy_sz': {
 'extra_args': {},
 'baos': True
 }
 },
 'likelihood': {
 'act_dr6_lenslike.ACTOR6LensLike': {
 'mock': False,
 'nsims_act': 792.0,
 'nsims_planck': 400.0,
 'no_like_corrections': True,
 'lens_only': True,
 'trim_lmax': 2998,
 'variant': 'actplanck_baseline',
 'apply_hartlap': True,
 'lamber': False,
 'nz': 100,
 'kmax': 10,
 'scale_cov': None,
 'type': [],
 'speed': -1,
 'stop_at_error': True,
 'version': None,
 'lmax': 4000,
 'input_params': [],
 'output_params': []
 }
 }
},
```

Write yaml

# Inference with agents

## Task 7: Reproduce the analysis - run mcmc

```
message=""" Run an MCMC analysis with cobaya.
1. Check whether the yaml file /Users/boris/CMBAgents/DataAgent/Coding/chains/dr6_lensing/dr6_lensing_rep.yaml exists.
 If it does not exist, ask admin for feedback.
2. Ask cobaya_agent how to run the mcmc.
 then ask admin for feedback.
3. Run the command in bash.
 Start with engineer.
"""
```

# Inference with agents

## Task 7: Reproduce the analysis - run mcmc

```
message=""
Run an MCMC analysis with cobaya.
1. Check whether the yaml file /Users/boris/CMBAgents/DataAgent/Coding/chains/dr6_lensing/dr6_lensing_rep.yaml exists.
 If it does not exist, ask admin for feedback.
2. Ask cobaya_agent how to run the mcmc.
 then ask admin for feedback.
3. Run the command in bash.
Start with engineer.
""
```

Next speaker: executor

>>>>>> EXECUTING CODE BLOCK (inferred language is bash)...  
 executor (to chat\_manager):

```
exitcode: 0 (execution succeeded)
Code output: /Users/boris/opt/miniconda3/lib/python3.9/site-packages/cosmopower/cosmopower_NN.py:336: RuntimeWarning: overflow encountered in exp
layers.append((self.betas_[i] + (1-self.betas_[i]))*(1/(1.+np.exp(-self.alphas_[i]*act[-1])))*act[-1])
[0 : output] Output to be read-from/written-into folder '.', with prefix 'dr6_lensing_rep'
[1 : classy_szf.classy_sz.classy_sz] Initialized!
[3 : classy_szf.classy_sz.classy_sz] Initialized!
[2 : classy_szf.classy_sz.classy_sz] Initialized!
[0 : classy_szf.classy_sz.classy_sz] Initialized!
[1 : bao.sdss_dr12_lrg_bao_dmdh] Initialized.
[2 : bao.sdss_dr12_lrg_bao_dmdh] Initialized.
[3 : bao.sdss_dr12_lrg_bao_dmdh] Initialized.
[0 : bao.sdss_dr12_lrg_bao_dmdh] Initialized.
[1 : bao.sdss_dr16_lrg_bao_dmdh] Initialized.
[2 : bao.sdss_dr16_lrg_bao_dmdh] Initialized.
[3 : bao.sdss_dr16_lrg_bao_dmdh] Initialized.
[0 : bao.sdss_dr16_lrg_bao_dmdh] Initialized.
[0 : bao.sixdf_2011_bao] Initialized.
[2 : bao.sixdf_2011_bao] Initialized.
[3 : bao.sixdf_2011_bao] Initialized.
[1 : bao.sixdf_2011_bao] Initialized.
[1 : mcmc] Getting initial point... (this may take a few seconds)
[2 : mcmc] Getting initial point... (this may take a few seconds)
[0 : mcmc] Getting initial point... (this may take a few seconds)
[3 : mcmc] Getting initial point... (this may take a few seconds)
[2 : mcmc] Initial point: H0:66.24648, logA:3.049948, ns:0.9704928, ombh2:0.02228236, omch2:0.118627
[1 : mcmc] Initial point: H0:65.84204, logA:3.049438, ns:0.9659865, ombh2:0.02238735, omch2:0.1193932
[0 : mcmc] Initial point: H0:67.98848, logA:3.051648, ns:0.961265, ombh2:0.0224652, omch2:0.1175497
[3 : mcmc] Initial point: H0:65.99235, logA:3.048629, ns:0.9689752, ombh2:0.02254777, omch2:0.1207122
[0 : mode] Measuring speeds... (this may take a few seconds)
[0 : mode] Setting measured speeds (per sec): (act_dr6_lensLike.ACTDR6LensLike: 1170.0, bao.sdss_dr12_lrg_bao_dmdh: 4060.0, bao.sdss_dr16_lrg_bao_dmdh: 11100.0, bao.sdss_dr7_mgs: 10500.0, bao.sixdf_2011_bao: 12000.0, classy_szf.classy_sz.classy_sz: 21.1)
```



Execute



# Inference with agents

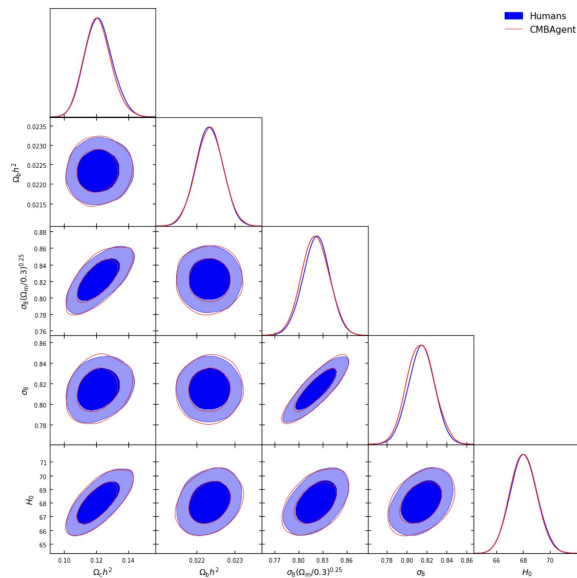
## Task 8: Plot contours against each other

```
message="" On the same plot, plot getdist contours for omch2, ombh2, $\sigma_8(\Omega_m/0.3)^{0.25}$, σ_8 , and H_0 ,
for chains "/Users/boris/CMBAgents/DataAgent/Coding/chains/dr6_lensing/lcdm_actplanck_baseline_167926925701" (label: "Humans")
and "/Users/boris/CMBAgents/DataAgent/Coding/generated_codes/dr6_lensing_rep" (label: "CMBAgent")
```

1. Make sure to use method with loadMCSamples (not MCSamples).
2. Remove 15% of burn-in.
3. Give me the 68%CL interval values on the parameters of interest but dont show them on the plot.
4. Write the code with engineer
5. Execute
6. Save the contour plot as /Users/boris/CMBAgents/DataAgent/Coding/chains/dr6\_lensing/dr6\_lensing\_baseline\_reproduction.png

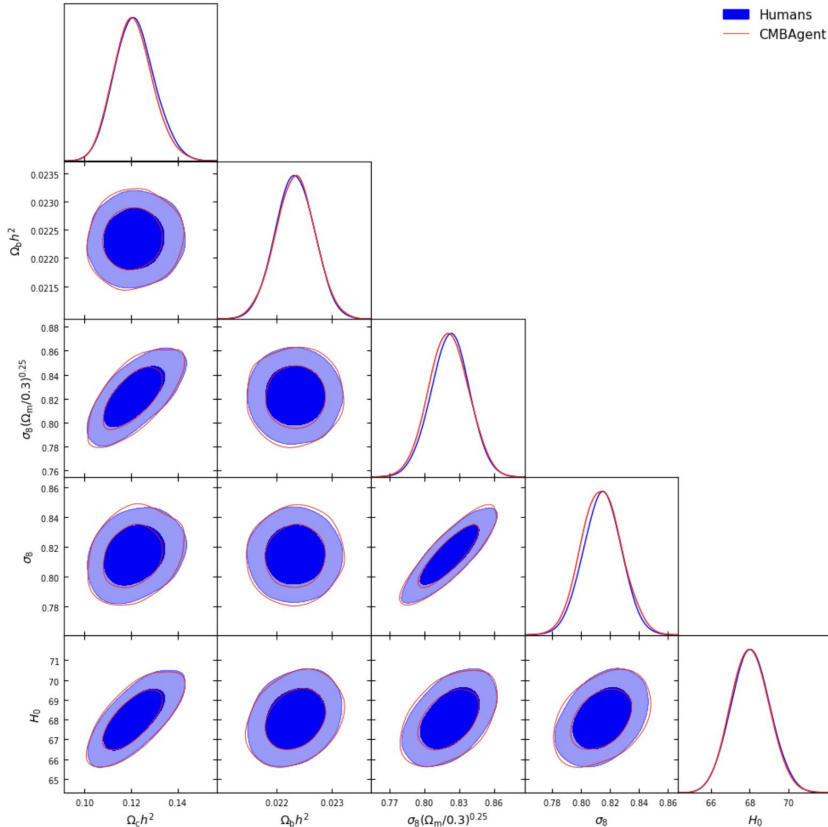
Start with getdit\_agent.

```
""""
```



Show results

# Inference with neural nets and agents



LLM-based agentic AI system running MCMCs with neural nets on your laptop.

Large portions of data analysis pipelines become automated in a fully controlled manner.

Can this change the way we do research?



**CMBAgent**  
*Stay tuned!*

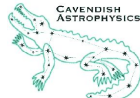
# Accelerated inference with neural networks and agents for Cosmic Microwave Background and Large Scale Structure analyses

Boris Bolliet

Cavendish Astrophysics and Kavli Institute for Cosmology, Cambridge

Work in collaboration with:

(Neural nets:) Kristen Surrao, Frank Qu, Hidde Jense, Colin Hill, Julien Lesgourgues, Alessio Spurio Mancini, Blake Sherwin  
(Agents:) Andrew Laverick, Inigo Zubeldia, Miles Cranmer, Julien Lesgourgues, Antony Lewis, Blake Sherwin



# Inference with agents

## Task 10: Plot TT spectra for varying fEDE

message="" Use class\_sz\_agent to make a plot of CMB TT spectra for 10 values of fEDE linearly operated between 0.001 and 0.5, for  $l$  between 2 and 8000.

1. Write the script and save the data.
2. Study the data to understand the dynamical range.
3. Set yaxis and xaxis limits based on dynamical range.
4. Save the results in a nicely presented plot with labels.
5. Give me the path to saved plot.

